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MODELING OF THE ELECTRO-CHEMICAL BEHAVIOR OF CHEMICALLY STIMULATED HYDROGEL LAYER SYSTEMS

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Summary: Hydrogels are viscoelastic electroactive polymers which respond to different external stimuli by a reversible change of volume through an uptake or delivery of surrounding water. Relevant stimuli include the change of pH, temperature, ion concentration, exposure to light, electrical and magnetic fields. Hydrogels also show a selective transport of ions if used as separation membranes.
The presented work provides the modeling of the transient electro-chemical behavior of hydrogel layer composites.
A chemically stimulated hydrogel layer system composed of two gels immersed in a solution bath containing mobile ions is analyzed. The modeling of the layer system is conducted for both anionic-anionic and anionic-cationic gel layers. An interlayer between the two gels is assumed and considered as an additional thin layer.
In order to numerically investigate the electro-chemical behavior of the hydrogel layer system, the finite element method is applied to the developed multifield formulation. The numerical simulation is realized by using one-dimensional, linear elements in space. To describe the occurring transport phenomena, the Poisson equation for the electrical field and the diffusion-migration-convection equations are fully coupled and solved simultaneously. The time discretization is performed using the implicit Euler method. As suitable initial condition a steady-state solution of the system is prescribed.
Results of the numerical simulation are the local concentrations of the mobile ions and the local electrical potential, which are determined at each time step as primary field variables. A nonzero volume charge density is observed in close proximity to the domain interfaces, whereas electroneutrality is obtained outside of the boundary regions. The nonzero charge density at the interfaces yields an electrical potential difference between gel and solution, consistent with the analytical solution of the Donnan potential.
The results give an insight into the occurring transport mechanisms and are in good agreement with previous works. For the application as membranes or sensors, (i) the swelling behavior and (ii) the permeability of the gel layer systems is of great interest. Since both are directly linked to the distribution of ions, which is provided by the described method, the present work is a relevant contribution towards these applications.